Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 02:56 AM EDT

PDB ID	:	3NRR
Title	:	Co-crystal structure of dihydrofolate reductase-thymidylate synthase from Babesia bovis with dUMP, Raltitrexed and NADP
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2010-06-30
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

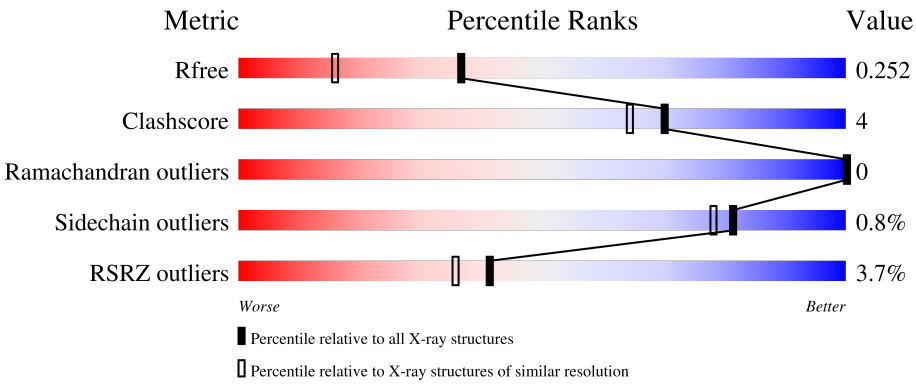
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	515	3% 91% 6% •
1	B	515	4% 92% 5% •

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9454 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	503	4013	2578	686	730	19	0	3	0
1	B	501	3991	2569	678	725	19	0	4	0

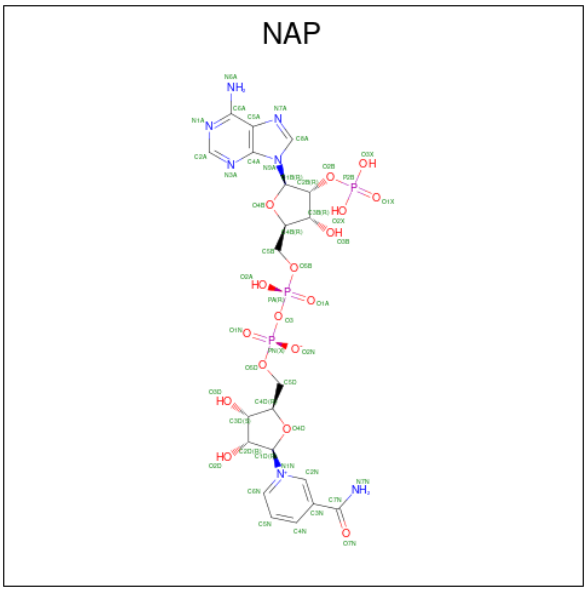
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A7ASX7
A	-2	PRO	-	expression tag	UNP A7ASX7
A	-1	GLY	-	expression tag	UNP A7ASX7
A	0	SER	-	expression tag	UNP A7ASX7
B	-3	GLY	-	expression tag	UNP A7ASX7
B	-2	PRO	-	expression tag	UNP A7ASX7
B	-1	GLY	-	expression tag	UNP A7ASX7
B	0	SER	-	expression tag	UNP A7ASX7

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

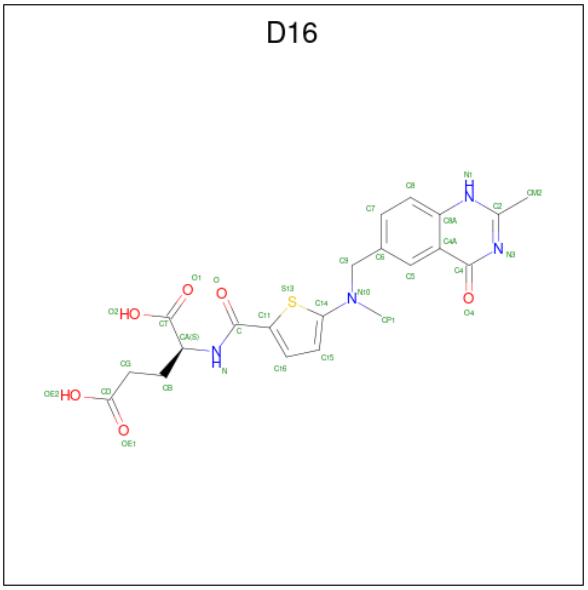
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	96	42	14	34	6	0	1
			Total	C	N	O	P		
3	B	1	96	42	14	34	6	0	1

- Molecule 4 is TOMUDEX (three-letter code: D16) (formula: $C_{21}H_{22}N_4O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	32	21	4	6	1	0	0
			Total	C	N	O	S		
4	A	1	32	21	4	6	1	0	0

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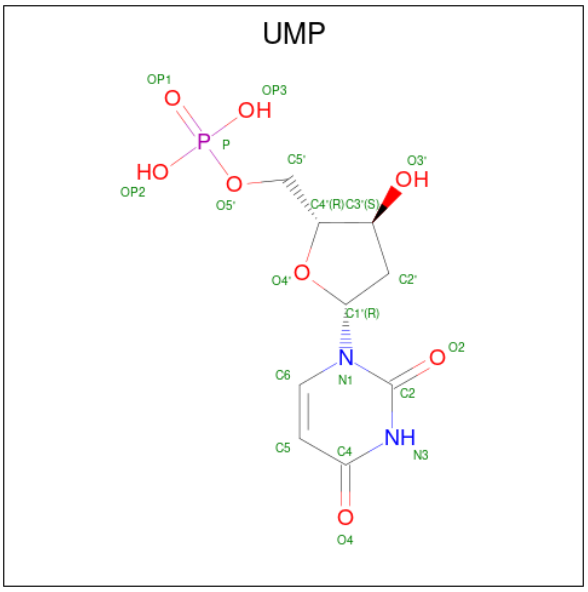
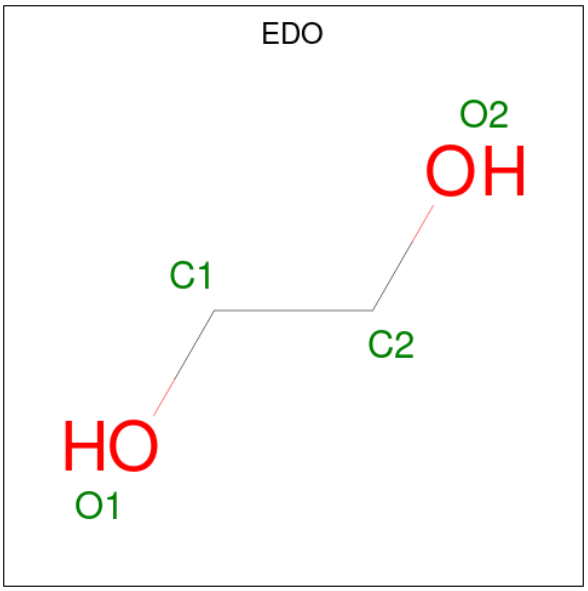
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	32	21	4	6	1	0	0
			Total	C	N	O	S		
4	B	1	32	21	4	6	1	0	0

- Molecule 5 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



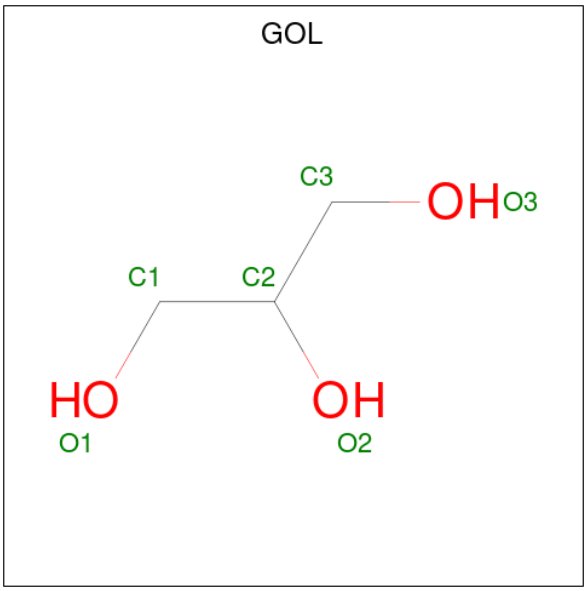
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	20	9	2	8	1	0	0
			Total	C	N	O	P		
5	B	1	20	9	2	8	1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



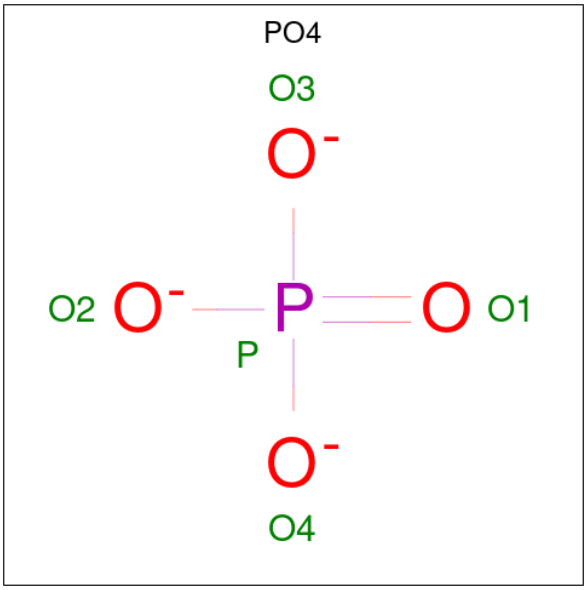
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	6	3	3	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
8	B	1	5	4	1	0	0

- Molecule 9 is water.

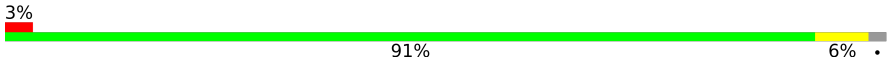
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	537	537	537	0	0
			Total	O		
9	B	488	488	488	0	0

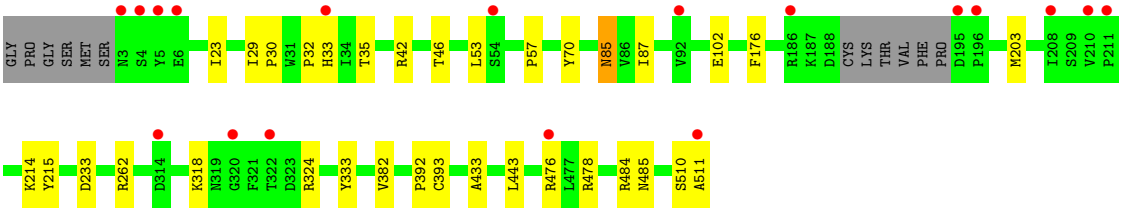
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Dihydrofolate reductase-thymidylate synthase

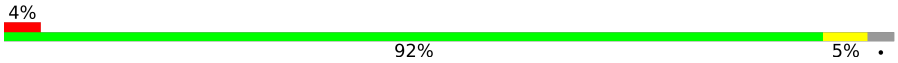
Chain A:

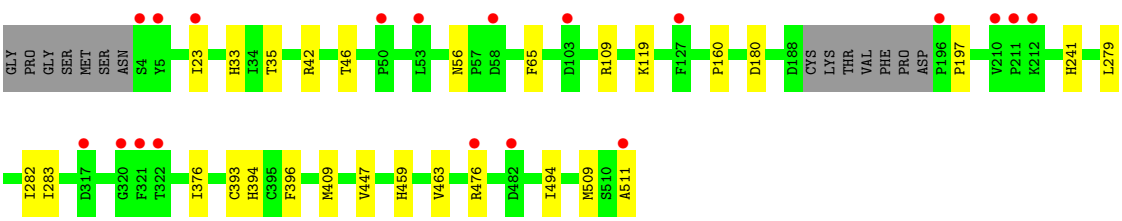




- Molecule 1: Dihydrofolate reductase-thymidylate synthase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.33Å 83.83Å 83.92Å 119.61° 102.04° 90.26°	Depositor
Resolution (Å)	19.94 – 1.80 19.94 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-1.80) 98.5 (19.94-1.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.236 0.209 , 0.252	Depositor DCC
R_{free} test set	5573 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,k,-k-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9454	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, EDO, D16, CL, UMP, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.72	0/4127	0.78	3/5617 (0.1%)
1	B	0.77	1/4108 (0.0%)	0.78	2/5593 (0.0%)
All	All	0.75	1/8235 (0.0%)	0.78	5/11210 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	394	HIS	C-O	-5.12	1.13	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	MET	CG-SD-CE	-5.96	90.66	100.20
1	B	180	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	396	PHE	N-CA-CB	-5.35	100.96	110.60
1	A	324	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	233	ASP	CB-CG-OD2	-5.02	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4013	0	3931	29	0
1	B	3991	0	3910	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	96	0	50	3	0
3	B	96	0	50	2	0
4	A	64	0	40	4	0
4	B	64	0	40	4	0
5	A	20	0	11	2	0
5	B	20	0	11	2	0
6	A	32	0	48	1	0
6	B	20	0	30	3	0
7	A	6	0	8	0	0
8	B	5	0	0	0	0
9	A	537	0	0	5	0
9	B	488	0	0	5	0
All	All	9454	0	8129	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:CYS:SG	5:A:525:UMP:C6	2.39	1.16
1:B:393:CYS:SG	5:B:525:UMP:C6	2.51	1.04
1:B:476[B]:ARG:HG2	1:B:476[B]:ARG:HH21	1.29	0.96
1:A:476[B]:ARG:HG2	1:A:476[B]:ARG:HH11	1.44	0.83
1:A:511:ALA:HB3	9:A:879:HOH:O	1.86	0.76
1:B:511:ALA:HB2	9:B:995:HOH:O	1.89	0.73
1:B:476[B]:ARG:HG2	1:B:476[B]:ARG:NH2	2.03	0.68
1:A:393:CYS:SG	5:A:525:UMP:C5	2.87	0.67
1:B:511:ALA:CB	9:B:995:HOH:O	2.43	0.66
1:A:33:HIS:CE1	1:A:35:THR:HG22	2.30	0.65
4:B:520:D16:C7	4:B:520:D16:HP13	2.27	0.64
4:A:520:D16:C7	4:A:520:D16:HP13	2.27	0.63
1:A:476[B]:ARG:HG2	1:A:476[B]:ARG:NH1	2.09	0.63
1:B:393:CYS:SG	5:B:525:UMP:C5	2.92	0.62
1:B:33:HIS:CE1	1:B:35:THR:HG22	2.36	0.60
1:A:510:SER:O	1:A:511:ALA:CB	2.48	0.60
1:B:476[B]:ARG:HD3	9:B:910:HOH:O	2.02	0.58
1:B:459:HIS:O	1:B:463[A]:VAL:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:MET:SD	1:B:511:ALA:OXT	2.64	0.55
1:A:23:ILE:O	3:A:515[B]:NAP:H2N	2.07	0.54
1:A:23:ILE:O	3:A:515[A]:NAP:H2N	2.08	0.54
1:A:510:SER:O	1:A:511:ALA:HB3	2.09	0.52
1:A:433:ALA:HA	1:A:443:LEU:HD21	1.92	0.51
1:A:32:PRO:HB2	1:A:176:PHE:CZ	2.46	0.51
1:A:102:GLU:O	3:A:515[B]:NAP:H2A	2.11	0.51
4:B:520:D16:C7	4:B:520:D16:CP1	2.89	0.50
4:A:520:D16:C7	4:A:520:D16:CP1	2.90	0.50
1:B:197:PRO:HG2	9:B:944:HOH:O	2.11	0.50
1:A:215:TYR:HA	6:A:532:EDO:H22	1.93	0.49
1:A:214:LYS:HG2	1:A:215:TYR:CE1	2.47	0.49
1:A:511:ALA:HB1	9:A:666:HOH:O	2.12	0.48
1:A:42:ARG:O	1:A:46:THR:HG23	2.13	0.48
1:B:23:ILE:O	3:B:515[A]:NAP:H2N	2.13	0.48
1:B:23:ILE:O	3:B:515[B]:NAP:H2N	2.13	0.48
1:A:478[A]:ARG:HD3	9:A:786:HOH:O	2.13	0.48
4:A:520:D16:HP13	4:A:520:D16:H7	1.95	0.48
4:B:520:D16:HP13	4:B:520:D16:H7	1.95	0.47
1:A:85:ASN:HD22	1:A:85:ASN:N	2.13	0.47
1:A:33:HIS:HE1	1:A:35:THR:HG22	1.76	0.47
4:B:520:D16:CP1	4:B:520:D16:H7	2.45	0.46
1:A:485:ASN:HB3	9:A:539:HOH:O	2.14	0.46
1:B:109:ARG:NE	6:B:537:EDO:O2	2.45	0.46
1:A:476[B]:ARG:HH11	1:A:476[B]:ARG:CG	2.22	0.46
1:A:70:TYR:CD2	1:A:87:ILE:HD11	2.52	0.45
1:B:376:ILE:O	6:B:532:EDO:H22	2.16	0.45
4:A:520:D16:CP1	4:A:520:D16:H7	2.48	0.43
1:A:53:LEU:O	1:A:57:PRO:HA	2.18	0.43
1:B:42:ARG:O	1:B:46:THR:HG23	2.18	0.43
1:B:409:MET:HA	1:B:447:VAL:O	2.19	0.42
1:A:511:ALA:HB2	9:A:994:HOH:O	2.19	0.42
1:B:283:ILE:HG23	1:B:494:ILE:HD13	2.03	0.41
1:B:476[B]:ARG:HH21	1:B:476[B]:ARG:CG	2.16	0.41
1:B:279:LEU:HA	1:B:282:ILE:HD12	2.01	0.41
1:A:29:ILE:HA	1:A:30:PRO:HD3	1.92	0.41
1:A:214:LYS:HG2	1:A:215:TYR:CD1	2.55	0.41
1:A:333:TYR:CE1	1:A:392:PRO:HB3	2.56	0.41
1:A:382:VAL:HG13	6:B:532:EDO:H11	2.03	0.40
1:B:119:LYS:HZ2	1:B:119:LYS:HG3	1.72	0.40
1:B:241:HIS:HD2	9:B:603:HOH:O	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/515 (98%)	492 (98%)	10 (2%)	0	100	100
1	B	501/515 (97%)	489 (98%)	12 (2%)	0	100	100
All	All	1003/1030 (97%)	981 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/460 (96%)	436 (99%)	4 (1%)	78	75
1	B	437/460 (95%)	434 (99%)	3 (1%)	84	81
All	All	877/920 (95%)	870 (99%)	7 (1%)	81	78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	262	ARG
1	A	318	LYS
1	A	484	ARG
1	B	56	ASN

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Mol	Chain	Res	Type
1	B	65	PHE
1	B	160	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	A	534	-	3,3,3	0.67	0	2,2,2	0.15	0
6	EDO	A	514	-	3,3,3	0.47	0	2,2,2	0.29	0
3	NAP	B	515[A]	-	45,52,52	0.84	1 (2%)	56,80,80	1.21	5 (8%)
6	EDO	B	539	-	3,3,3	0.56	0	2,2,2	0.22	0
3	NAP	A	515[A]	-	45,52,52	0.89	1 (2%)	56,80,80	1.22	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	PO4	B	513	-	4,4,4	0.95	0	6,6,6	0.52	0
6	EDO	A	533	-	3,3,3	0.52	0	2,2,2	0.10	0
5	UMP	B	525	-	21,21,21	1.20	2 (9%)	31,31,31	1.22	3 (9%)
6	EDO	B	537	-	3,3,3	0.45	0	2,2,2	0.31	0
7	GOL	A	540	-	5,5,5	0.21	0	5,5,5	0.54	0
5	UMP	A	525	-	21,21,21	0.97	2 (9%)	31,31,31	1.51	6 (19%)
6	EDO	A	537	-	3,3,3	0.46	0	2,2,2	0.19	0
6	EDO	B	533	-	3,3,3	0.36	0	2,2,2	0.45	0
4	D16	A	520	-	30,34,34	1.79	4 (13%)	37,48,48	1.79	10 (27%)
4	D16	A	530	-	30,34,34	1.59	5 (16%)	37,48,48	1.28	2 (5%)
3	NAP	B	515[B]	-	45,52,52	0.87	2 (4%)	56,80,80	1.15	4 (7%)
4	D16	B	530	-	30,34,34	1.47	4 (13%)	37,48,48	1.25	4 (10%)
6	EDO	A	536	-	3,3,3	0.44	0	2,2,2	0.19	0
4	D16	B	520	-	30,34,34	1.80	5 (16%)	37,48,48	1.69	8 (21%)
6	EDO	A	532	-	3,3,3	0.59	0	2,2,2	0.15	0
6	EDO	B	532	-	3,3,3	0.61	0	2,2,2	0.32	0
3	NAP	A	515[B]	-	45,52,52	0.85	1 (2%)	56,80,80	1.16	5 (8%)
6	EDO	A	531	-	3,3,3	0.74	0	2,2,2	0.61	0
6	EDO	B	534	-	3,3,3	0.47	0	2,2,2	0.29	0
6	EDO	A	535	-	3,3,3	0.43	0	2,2,2	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	534	-	-	1/1/1/1	-
6	EDO	A	514	-	-	0/1/1/1	-
3	NAP	B	515[A]	-	-	2/31/67/67	0/5/5/5
6	EDO	B	539	-	-	1/1/1/1	-
3	NAP	A	515[A]	-	-	1/31/67/67	0/5/5/5
6	EDO	A	533	-	-	1/1/1/1	-
5	UMP	B	525	-	-	1/10/22/22	0/2/2/2
6	EDO	B	537	-	-	1/1/1/1	-
7	GOL	A	540	-	-	2/4/4/4	-
5	UMP	A	525	-	-	1/10/22/22	0/2/2/2
6	EDO	A	537	-	-	0/1/1/1	-
6	EDO	B	533	-	-	1/1/1/1	-
4	D16	A	520	-	-	3/19/25/25	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	D16	A	530	-	-	6/19/25/25	0/3/3/3
3	NAP	B	515[B]	-	-	1/31/67/67	0/5/5/5
4	D16	B	530	-	-	5/19/25/25	0/3/3/3
6	EDO	A	536	-	-	0/1/1/1	-
4	D16	B	520	-	-	4/19/25/25	0/3/3/3
6	EDO	A	532	-	-	1/1/1/1	-
6	EDO	B	532	-	-	1/1/1/1	-
3	NAP	A	515[B]	-	-	2/31/67/67	0/5/5/5
6	EDO	A	531	-	-	0/1/1/1	-
6	EDO	B	534	-	-	1/1/1/1	-
6	EDO	A	535	-	-	0/1/1/1	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	520	D16	O4-C4	6.35	1.34	1.23
4	A	520	D16	O4-C4	5.95	1.34	1.23
4	A	530	D16	O4-C4	5.11	1.32	1.23
4	B	530	D16	O4-C4	4.60	1.31	1.23
4	A	520	D16	C4A-C8A	4.58	1.48	1.41
4	B	520	D16	C4A-C8A	4.38	1.48	1.41
4	A	530	D16	C4A-C8A	3.33	1.46	1.41
4	A	520	D16	C4-N3	-3.24	1.32	1.39
3	A	515[A]	NAP	C7N-N7N	-3.13	1.27	1.33
4	B	530	D16	C8A-N1	-3.06	1.34	1.39
4	B	520	D16	C4-N3	-3.06	1.32	1.39
3	A	515[B]	NAP	C7N-N7N	-3.05	1.27	1.33
4	B	530	D16	C4A-C8A	2.91	1.45	1.41
5	B	525	UMP	C6-C5	2.71	1.41	1.35
3	B	515[A]	NAP	C7N-N7N	-2.68	1.27	1.33
3	B	515[B]	NAP	C7N-N7N	-2.68	1.27	1.33
4	A	520	D16	C8A-N1	-2.60	1.35	1.39
5	A	525	UMP	C6-C5	2.53	1.40	1.35
4	A	530	D16	C8A-N1	-2.52	1.35	1.39
4	A	530	D16	C4-N3	-2.40	1.34	1.39
4	A	530	D16	OE1-CD	2.21	1.29	1.22
4	B	530	D16	C4-N3	-2.19	1.34	1.39
5	A	525	UMP	C5-C4	-2.08	1.39	1.43
5	B	525	UMP	P-OP2	-2.08	1.46	1.54
4	B	520	D16	C2-N3	2.04	1.36	1.31
4	B	520	D16	C8A-N1	-2.02	1.36	1.39
3	B	515[B]	NAP	O4B-C1B	2.01	1.43	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	530	D16	C6-C9-N10	-4.78	107.87	113.81
4	B	520	D16	CP1-N10-C14	-4.69	111.33	119.96
3	A	515[A]	NAP	N3A-C2A-N1A	-4.60	121.49	128.68
3	B	515[A]	NAP	N3A-C2A-N1A	-4.40	121.81	128.68
3	A	515[B]	NAP	N3A-C2A-N1A	-4.25	122.03	128.68
5	A	525	UMP	C2'-C1'-N1	4.22	123.49	113.77
3	B	515[B]	NAP	N3A-C2A-N1A	-4.18	122.14	128.68
4	B	530	D16	C8A-C4A-C4	-4.11	115.70	120.39
4	A	520	D16	CA-N-C	4.09	131.62	121.60
4	B	520	D16	C8A-C4A-C4	-3.59	116.30	120.39
4	A	520	D16	C7-C6-C5	3.39	123.29	118.54
4	A	520	D16	C4A-C5-C6	-3.34	116.11	121.41
5	A	525	UMP	C5-C4-N3	3.26	119.72	114.84
4	B	520	D16	C4A-C5-C6	-3.17	116.37	121.41
4	A	530	D16	C8A-C4A-C4	-3.17	116.77	120.39
4	B	520	D16	C5-C4A-C8A	3.13	121.80	119.00
4	B	530	D16	C6-C9-N10	-3.11	109.95	113.81
4	A	520	D16	CP1-N10-C14	-3.09	114.29	119.96
4	A	520	D16	C6-C9-N10	-3.06	110.01	113.81
5	B	525	UMP	C2'-C1'-N1	3.06	120.82	113.77
4	A	520	D16	C5-C4A-C8A	3.02	121.70	119.00
4	B	520	D16	C6-C9-N10	-2.95	110.15	113.81
5	A	525	UMP	C4-N3-C2	-2.91	122.74	126.58
5	B	525	UMP	C5-C4-N3	2.85	119.10	114.84
3	B	515[A]	NAP	O7N-C7N-C3N	-2.84	116.23	119.63
3	B	515[B]	NAP	O7N-C7N-C3N	-2.83	116.25	119.63
4	A	520	D16	C8A-C4A-C4	-2.80	117.20	120.39
3	A	515[A]	NAP	O7N-C7N-C3N	-2.77	116.32	119.63
4	A	520	D16	O-C-N	2.71	127.43	122.45
3	B	515[A]	NAP	C3N-C7N-N7N	2.70	121.00	117.75
3	B	515[B]	NAP	C3N-C7N-N7N	2.70	121.00	117.75
3	A	515[B]	NAP	O7N-C7N-C3N	-2.66	116.45	119.63
4	B	520	D16	O4-C4-N3	2.63	123.72	120.59
4	B	520	D16	C7-C6-C5	2.62	122.21	118.54
5	B	525	UMP	C6-C5-C4	-2.53	116.06	119.52
3	A	515[A]	NAP	O2B-P2B-O1X	-2.51	99.70	109.39
3	B	515[A]	NAP	O3X-P2B-O2X	2.45	116.98	107.64
3	B	515[B]	NAP	O3X-P2B-O2X	2.39	116.79	107.64
3	A	515[A]	NAP	C3N-C7N-N7N	2.38	120.61	117.75
3	A	515[B]	NAP	C3N-C7N-N7N	2.38	120.61	117.75
5	A	525	UMP	N3-C2-N1	2.29	117.93	114.89
3	A	515[A]	NAP	O3X-P2B-O2X	2.24	116.21	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	525	UMP	OP3-P-OP2	2.16	115.88	107.64
3	B	515[A]	NAP	C4A-C5A-N7A	-2.15	107.16	109.40
4	A	520	D16	O4-C4-N3	2.14	123.14	120.59
3	A	515[B]	NAP	O3X-P2B-O2X	2.14	115.83	107.64
4	B	520	D16	O4-C4-C4A	-2.13	118.28	121.54
4	B	530	D16	C5-C4A-C8A	2.06	120.85	119.00
5	A	525	UMP	P-O5'-C5'	2.06	123.98	118.30
4	B	530	D16	O4-C4-N3	-2.06	118.15	120.59
4	A	520	D16	CT-CA-N	2.02	115.34	110.55
3	A	515[B]	NAP	O2A-PA-O1A	2.01	122.16	112.24

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	520	D16	CT-CA-CB-CG
7	A	540	GOL	O2-C2-C3-O3
7	A	540	GOL	C1-C2-C3-O3
4	A	530	D16	N-CA-CB-CG
6	A	532	EDO	O1-C1-C2-O2
6	B	539	EDO	O1-C1-C2-O2
6	B	537	EDO	O1-C1-C2-O2
6	A	534	EDO	O1-C1-C2-O2
4	A	530	D16	C6-C9-N10-CP1
4	B	530	D16	C6-C9-N10-CP1
4	B	520	D16	N-CA-CB-CG
4	A	530	D16	CT-CA-CB-CG
6	A	533	EDO	O1-C1-C2-O2
6	B	532	EDO	O1-C1-C2-O2
4	A	520	D16	CA-CB-CG-CD
3	B	515[A]	NAP	C2B-O2B-P2B-O3X
6	B	534	EDO	O1-C1-C2-O2
4	B	530	D16	CT-CA-CB-CG
3	A	515[A]	NAP	C4D-C5D-O5D-PN
3	A	515[B]	NAP	C4D-C5D-O5D-PN
4	A	520	D16	OE2-CD-CG-CB
3	B	515[A]	NAP	C4D-C5D-O5D-PN
4	B	530	D16	OE1-CD-CG-CB
4	A	520	D16	OE1-CD-CG-CB
3	B	515[B]	NAP	C4D-C5D-O5D-PN
4	A	530	D16	C5-C6-C9-N10
4	B	530	D16	OE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
6	B	533	EDO	O1-C1-C2-O2
4	A	530	D16	OE1-CD-CG-CB
4	A	530	D16	OE2-CD-CG-CB
4	B	520	D16	OE2-CD-CG-CB
3	A	515[B]	NAP	C2B-O2B-P2B-O2X
5	B	525	UMP	O4'-C4'-C5'-O5'
4	B	530	D16	N-CA-CB-CG
4	B	520	D16	OE1-CD-CG-CB
5	A	525	UMP	O4'-C4'-C5'-O5'

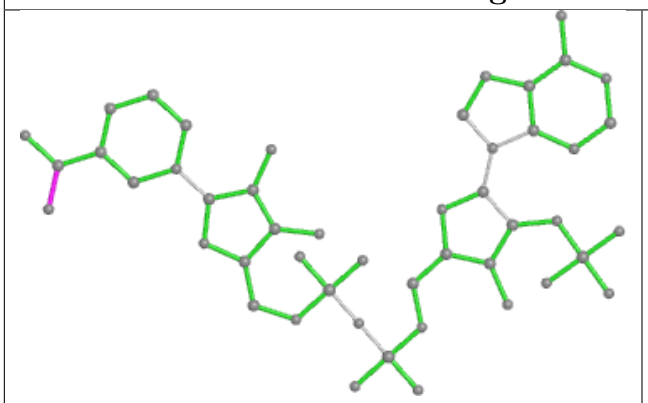
There are no ring outliers.

11 monomers are involved in 21 short contacts:

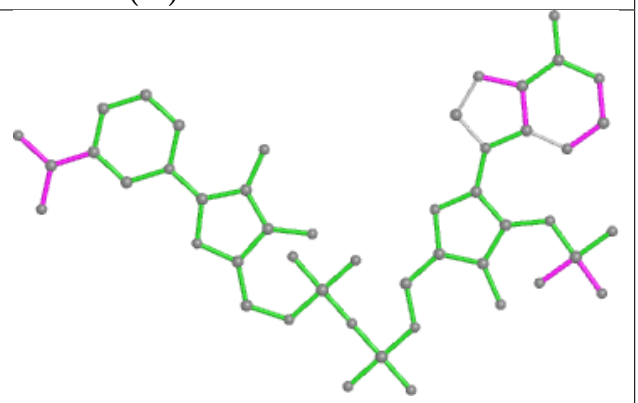
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	515[A]	NAP	1	0
3	A	515[A]	NAP	1	0
5	B	525	UMP	2	0
6	B	537	EDO	1	0
5	A	525	UMP	2	0
4	A	520	D16	4	0
3	B	515[B]	NAP	1	0
4	B	520	D16	4	0
6	A	532	EDO	1	0
6	B	532	EDO	2	0
3	A	515[B]	NAP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

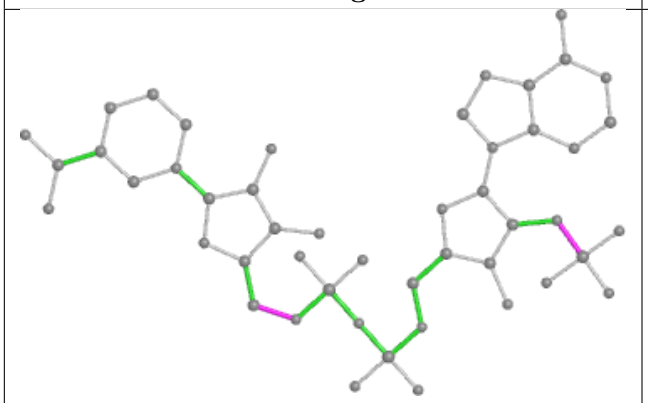
Ligand NAP B 515 (A)



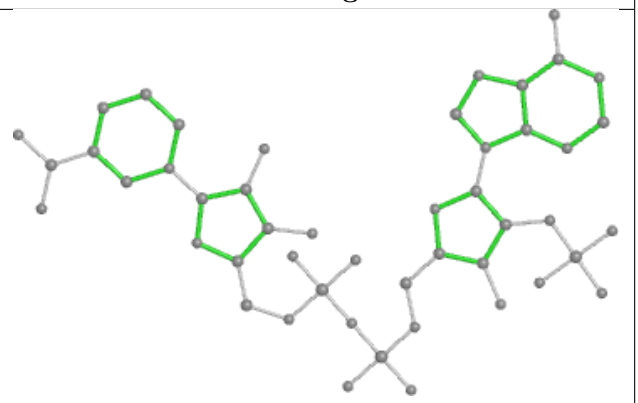
Bond lengths



Bond angles

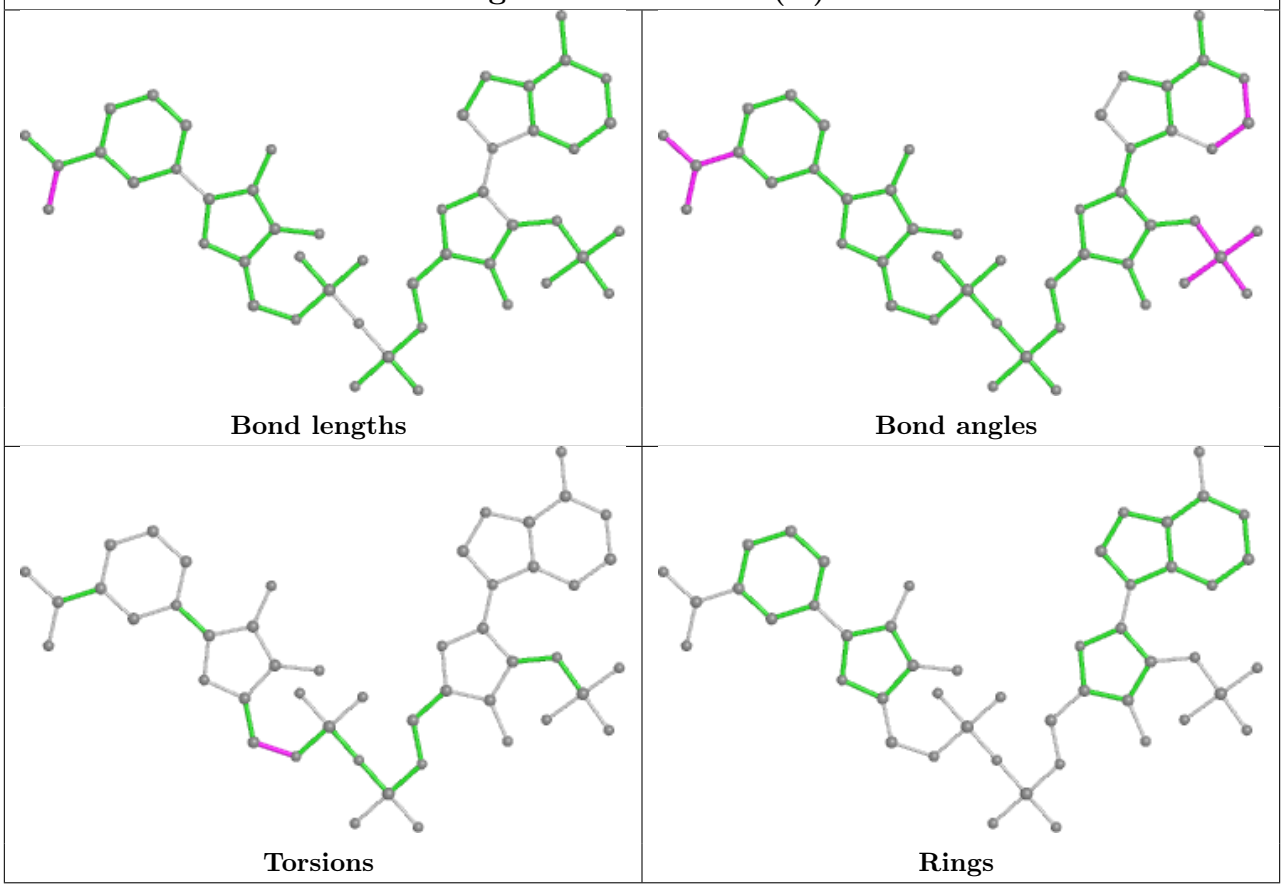


Torsions

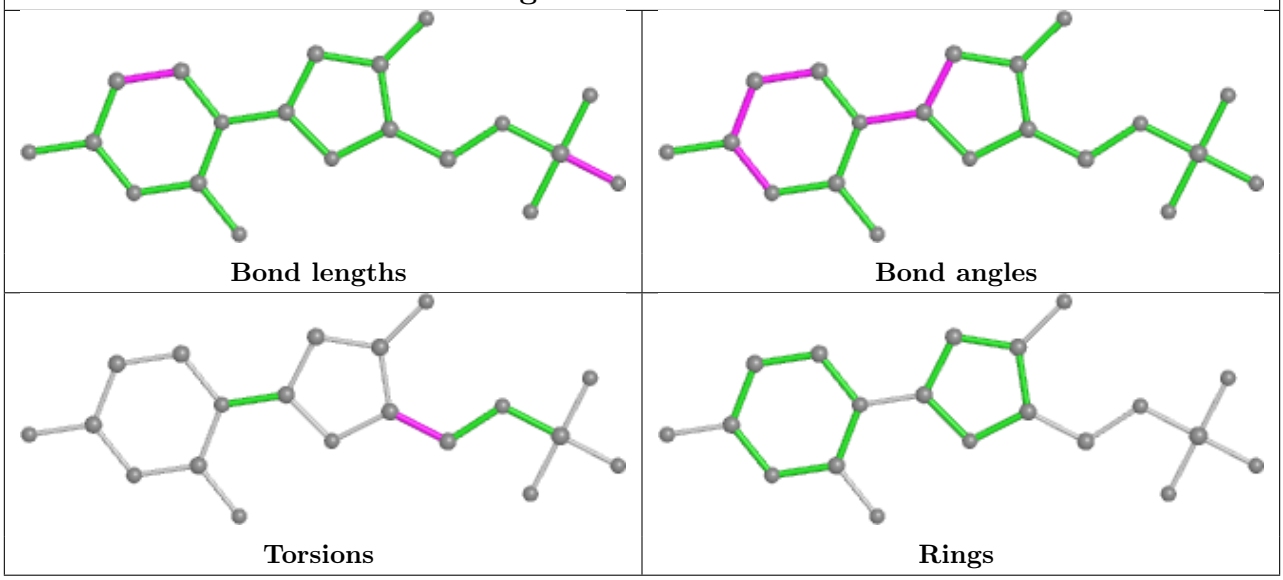


Rings

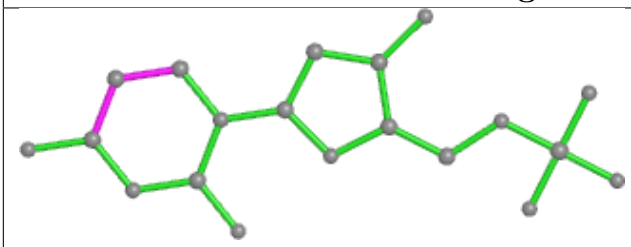
Ligand NAP A 515 (A)



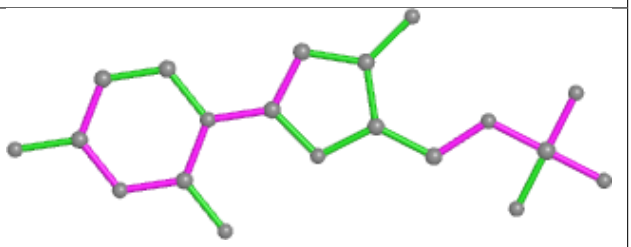
Ligand UMP B 525



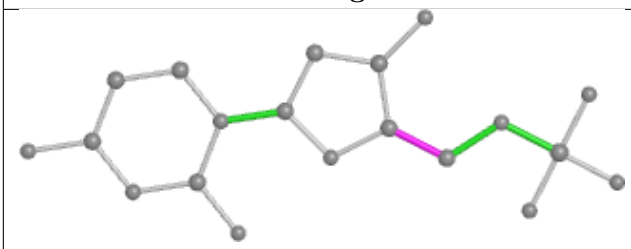
Ligand UMP A 525



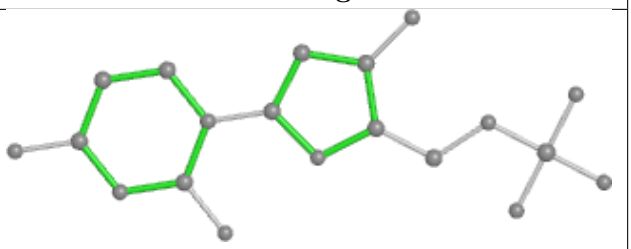
Bond lengths



Bond angles

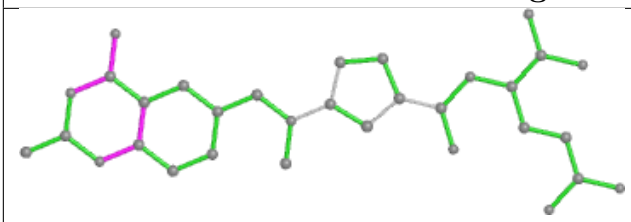


Torsions

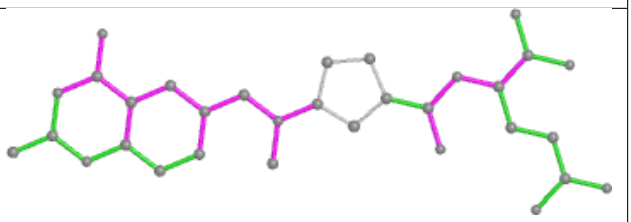


Rings

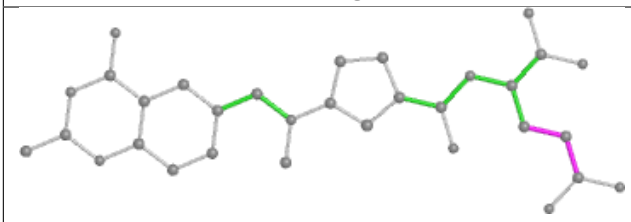
Ligand D16 A 520



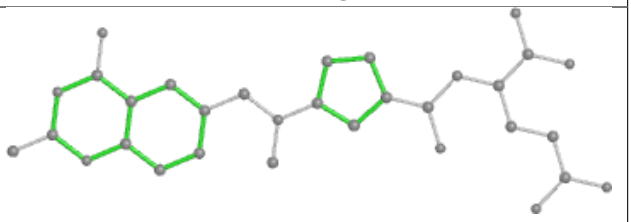
Bond lengths



Bond angles

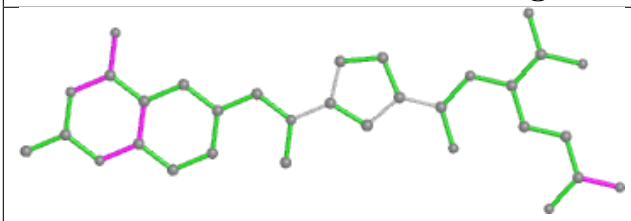


Torsions

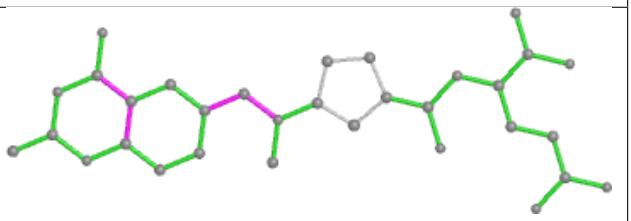


Rings

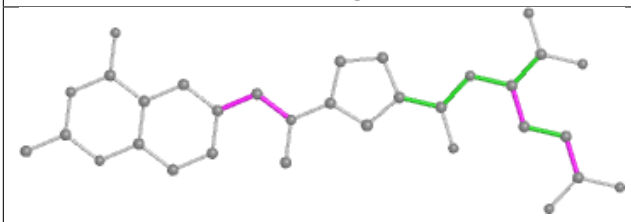
Ligand D16 A 530



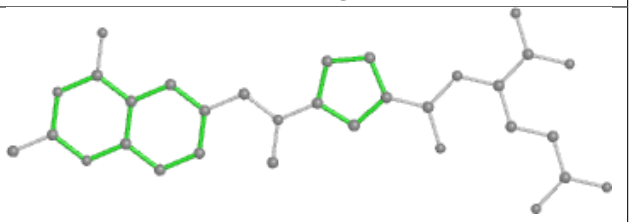
Bond lengths



Bond angles

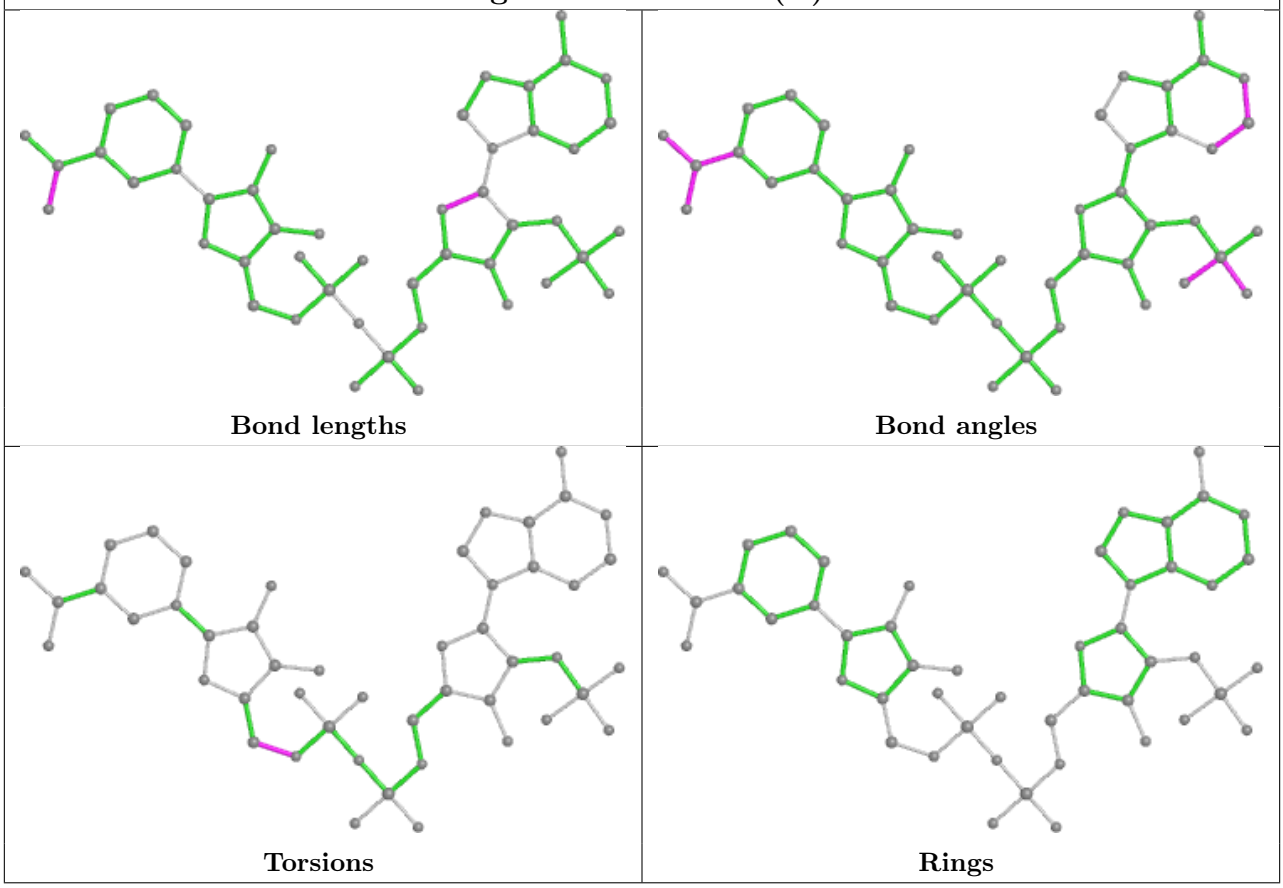


Torsions

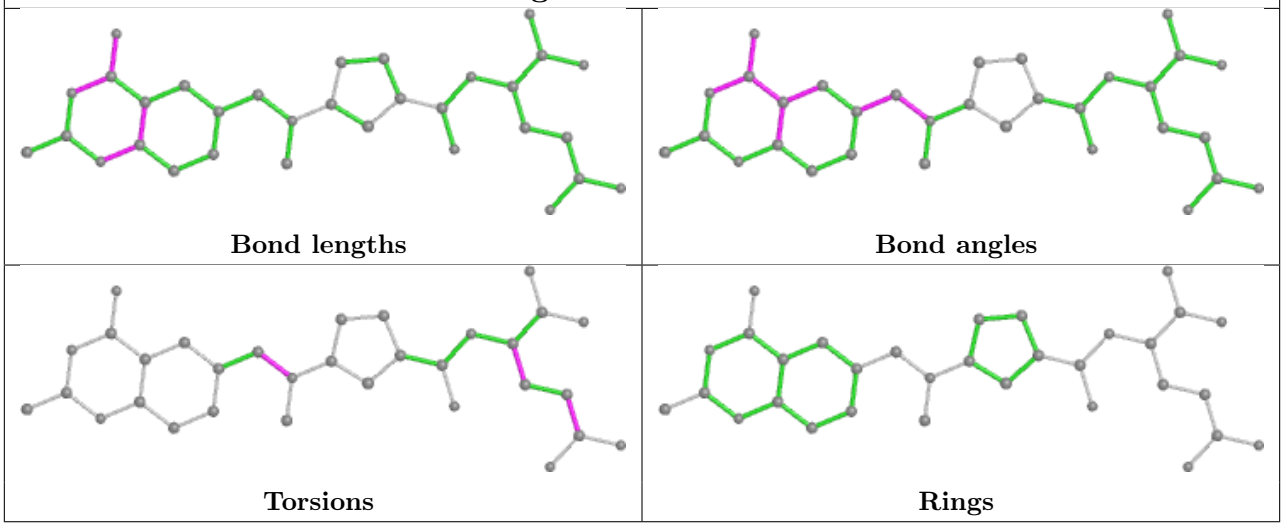


Rings

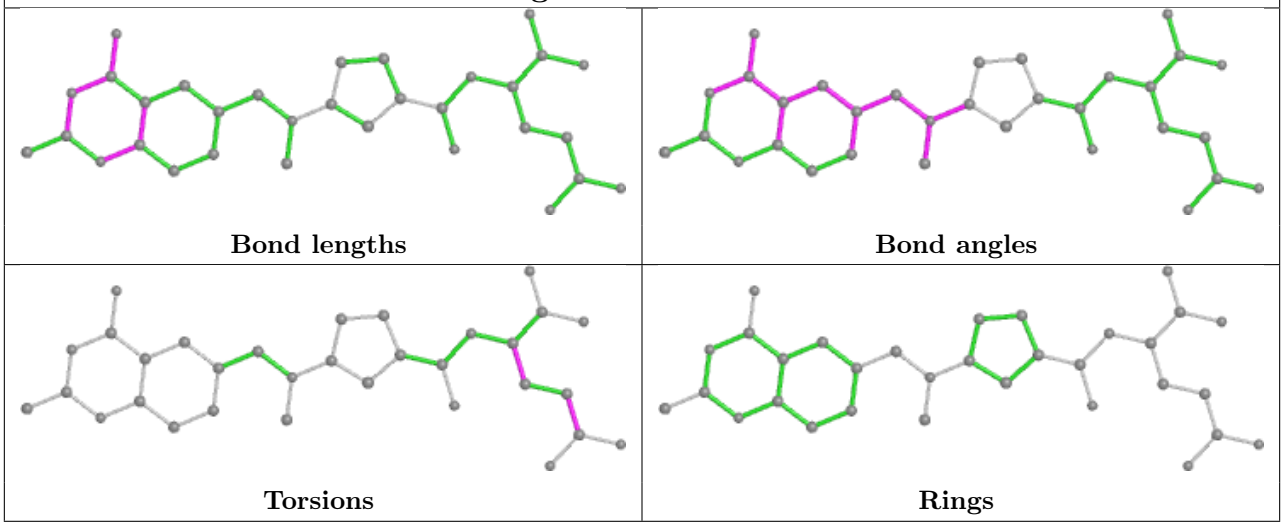
Ligand NAP B 515 (B)



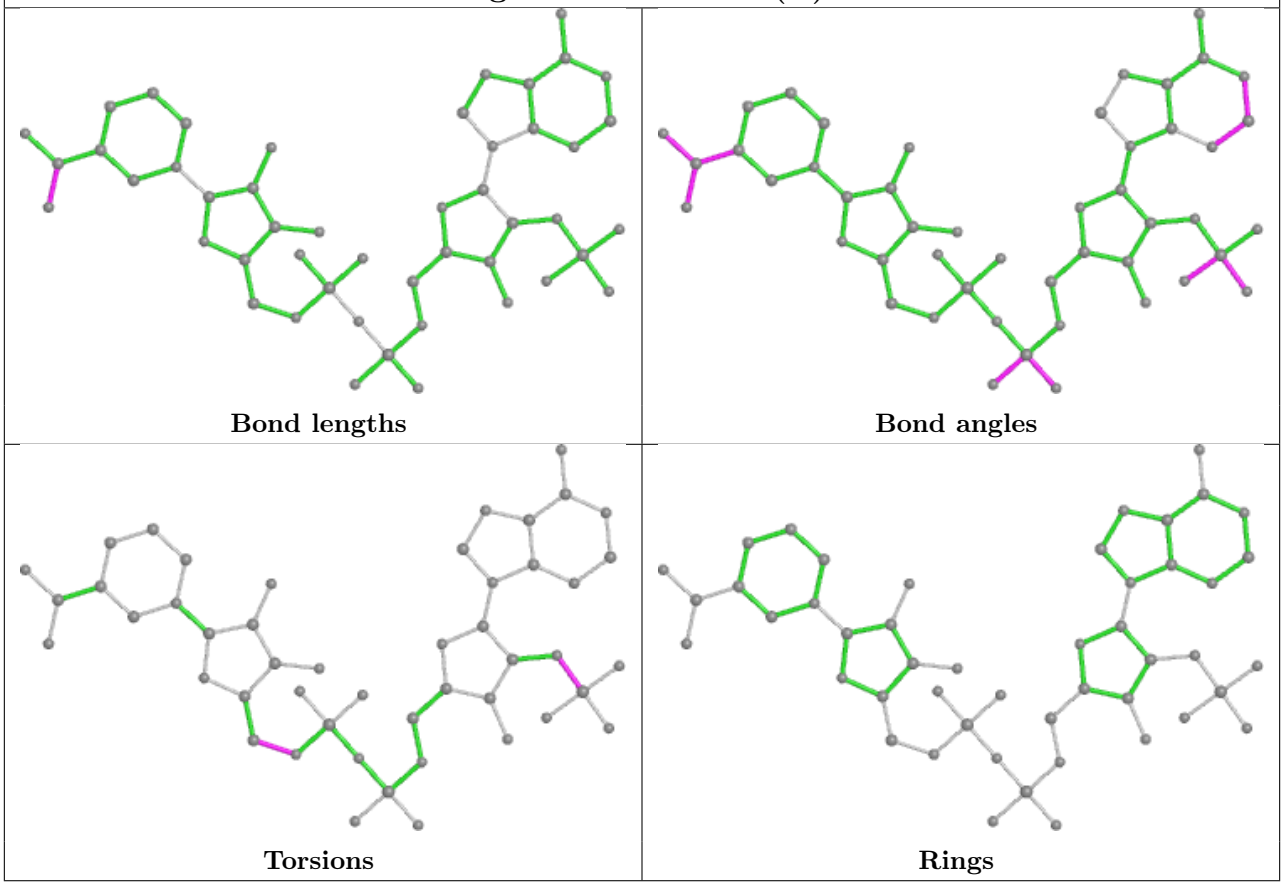
Ligand D16 B 530



Ligand D16 B 520



Ligand NAP A 515 (B)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	503/515 (97%)	0.22	18 (3%)	42	37	8, 16, 41, 79	0
1	B	501/515 (97%)	0.18	19 (3%)	40	35	7, 16, 39, 82	0
All	All	1004/1030 (97%)	0.20	37 (3%)	41	36	7, 16, 40, 82	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	ALA	7.6
1	B	511	ALA	6.8
1	A	211	PRO	5.6
1	B	210	VAL	5.1
1	A	210	VAL	4.9
1	B	211	PRO	4.6
1	B	322	THR	3.8
1	A	33	HIS	3.7
1	A	3	ASN	3.2
1	A	196	PRO	3.2
1	A	208	ILE	3.2
1	B	317	ASP	3.1
1	B	196	PRO	3.1
1	A	4	SER	3.1
1	A	322	THR	3.0
1	B	4	SER	3.0
1	A	92	VAL	2.8
1	B	5	TYR	2.8
1	A	6	GLU	2.6
1	B	50	PRO	2.6
1	A	476[A]	ARG	2.6
1	B	320	GLY	2.5
1	B	476[A]	ARG	2.5
1	A	320	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	5	TYR	2.4
1	A	314	ASP	2.3
1	B	23	ILE	2.2
1	B	53	LEU	2.2
1	B	482	ASP	2.2
1	A	186	ARG	2.1
1	B	127	PHE	2.1
1	A	195	ASP	2.1
1	B	212	LYS	2.1
1	A	54	SER	2.0
1	B	58	ASP	2.0
1	B	103	ASP	2.0
1	B	321	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	534	4/4	0.60	0.19	45,46,46,46	0
6	EDO	A	537	4/4	0.62	0.25	34,35,37,39	0
6	EDO	A	532	4/4	0.64	0.17	37,38,39,42	0
7	GOL	A	540	6/6	0.69	0.27	40,43,44,45	0
6	EDO	B	537	4/4	0.71	0.17	48,50,50,51	0
6	EDO	B	534	4/4	0.81	0.12	40,41,42,42	0
6	EDO	A	536	4/4	0.81	0.16	35,39,40,44	0
6	EDO	A	514	4/4	0.81	0.18	31,32,33,35	0
6	EDO	B	539	4/4	0.82	0.16	28,32,34,35	0
6	EDO	A	535	4/4	0.83	0.11	34,38,38,42	0

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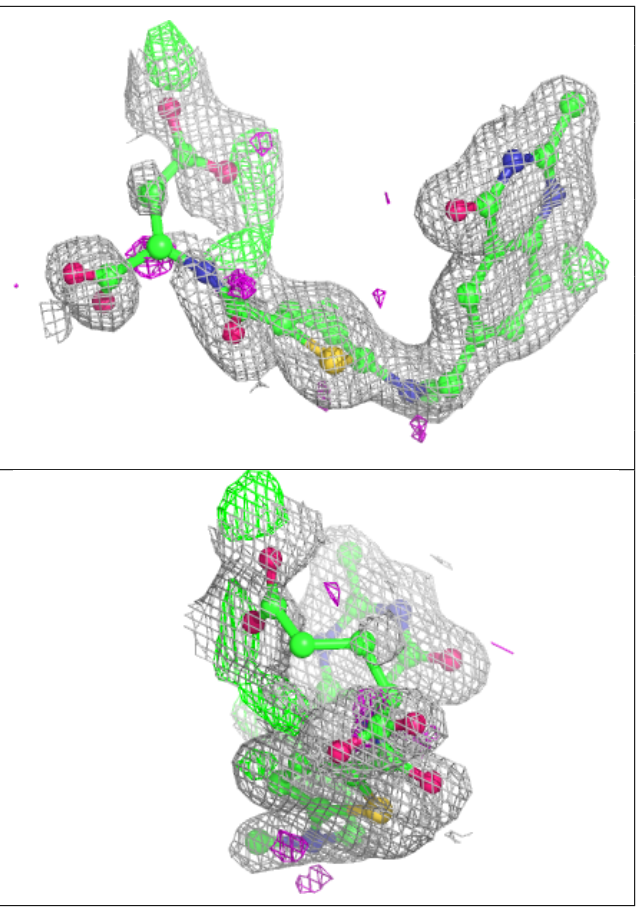
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	D16	A	520	32/32	0.83	0.18	16,25,48,50	0
8	PO4	B	513	5/5	0.84	0.30	47,51,52,53	0
6	EDO	A	531	4/4	0.86	0.13	25,25,27,31	0
4	D16	B	520	32/32	0.86	0.17	14,23,40,41	0
6	EDO	B	532	4/4	0.87	0.18	28,29,30,30	0
2	CL	B	514	1/1	0.89	0.17	54,54,54,54	0
4	D16	A	530	32/32	0.93	0.11	10,14,30,31	0
6	EDO	B	533	4/4	0.93	0.09	35,35,36,38	0
6	EDO	A	533	4/4	0.93	0.08	35,36,38,40	0
3	NAP	A	515[B]	48/48	0.94	0.12	13,20,30,32	48
3	NAP	A	515[A]	48/48	0.94	0.12	13,19,30,30	48
4	D16	B	530	32/32	0.94	0.12	10,14,32,35	0
3	NAP	B	515[B]	48/48	0.95	0.12	11,18,28,29	48
3	NAP	B	515[A]	48/48	0.95	0.12	11,18,26,27	48
2	CL	A	513	1/1	0.97	0.09	28,28,28,28	0
5	UMP	A	525	20/20	0.97	0.09	9,10,14,15	0
5	UMP	B	525	20/20	0.97	0.09	7,11,15,17	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

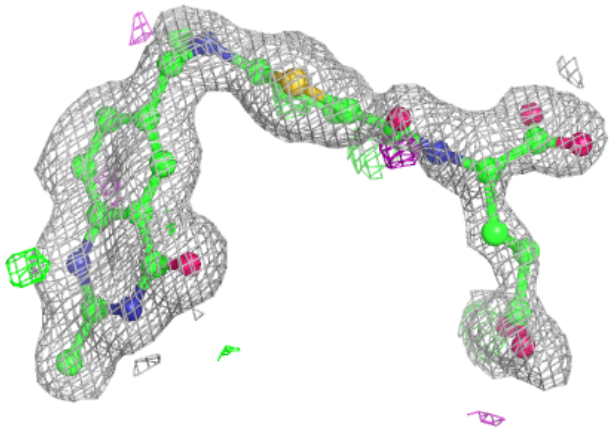
Electron density around D16 A 520:

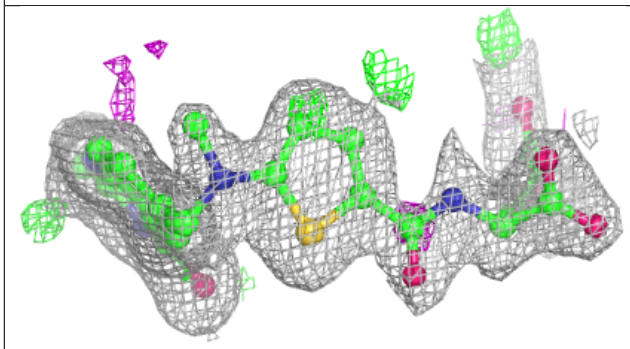
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

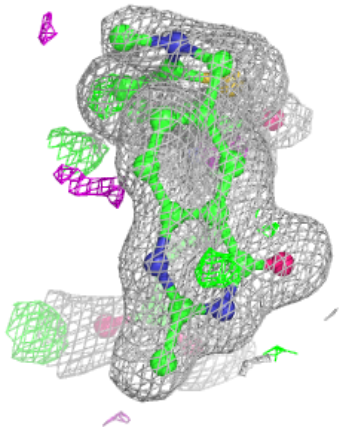


Electron density around D16 B 520:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

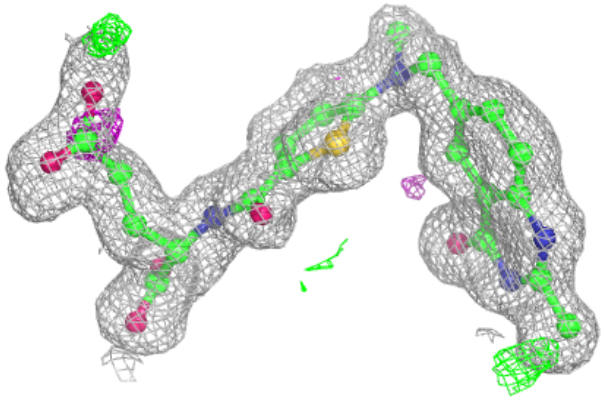


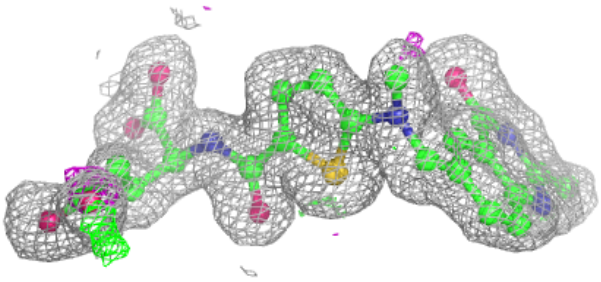


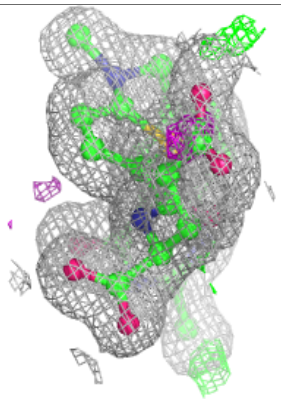


Electron density around D16 A 530:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

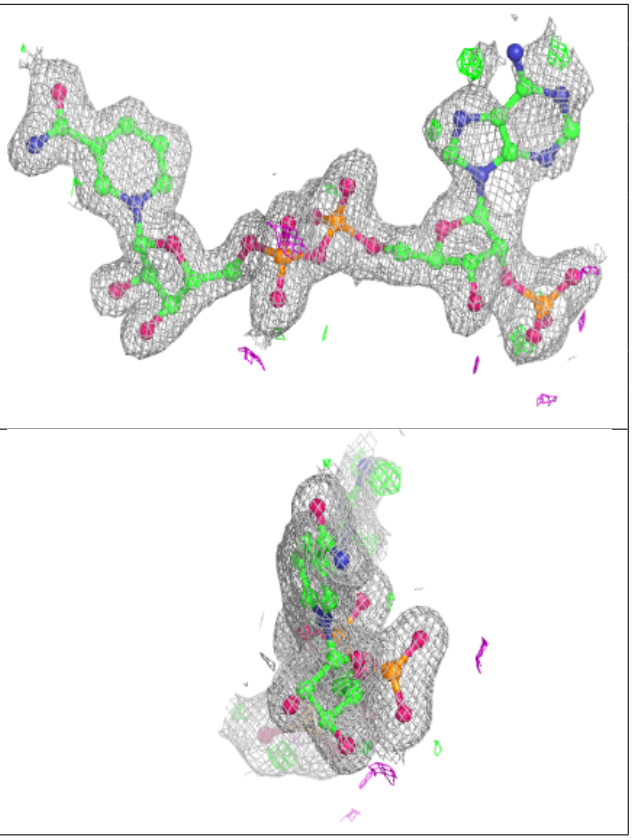


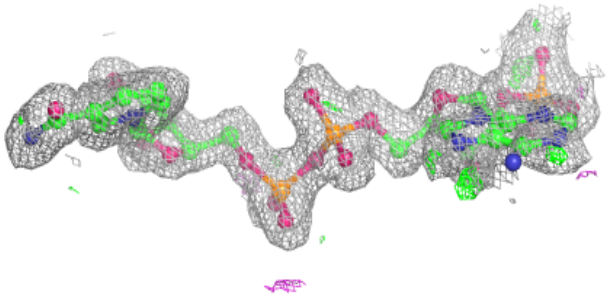




Electron density around NAP A 515 (B):

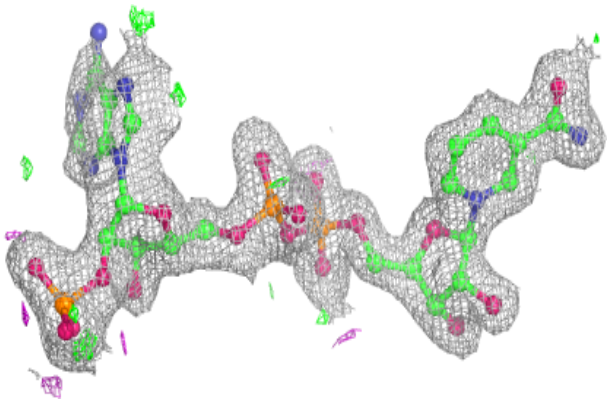
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

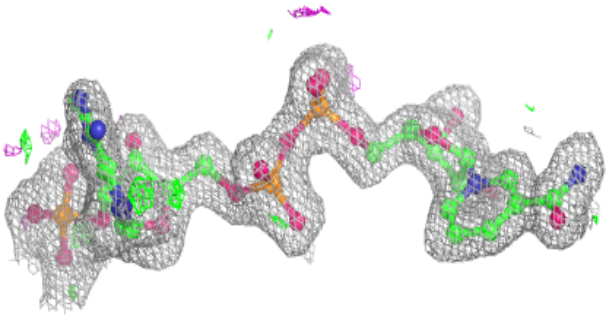


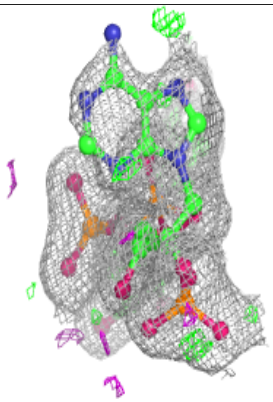


Electron density around NAP A 515 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

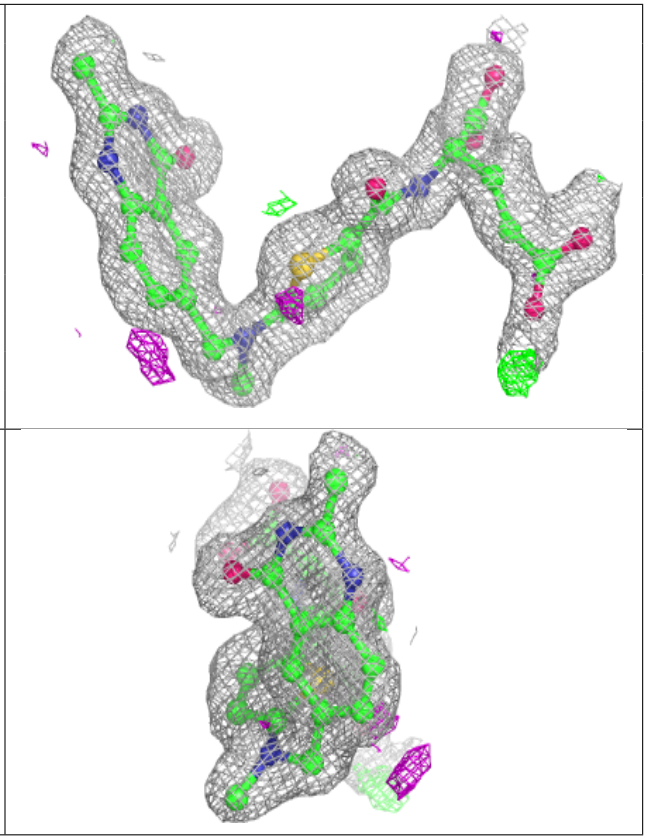






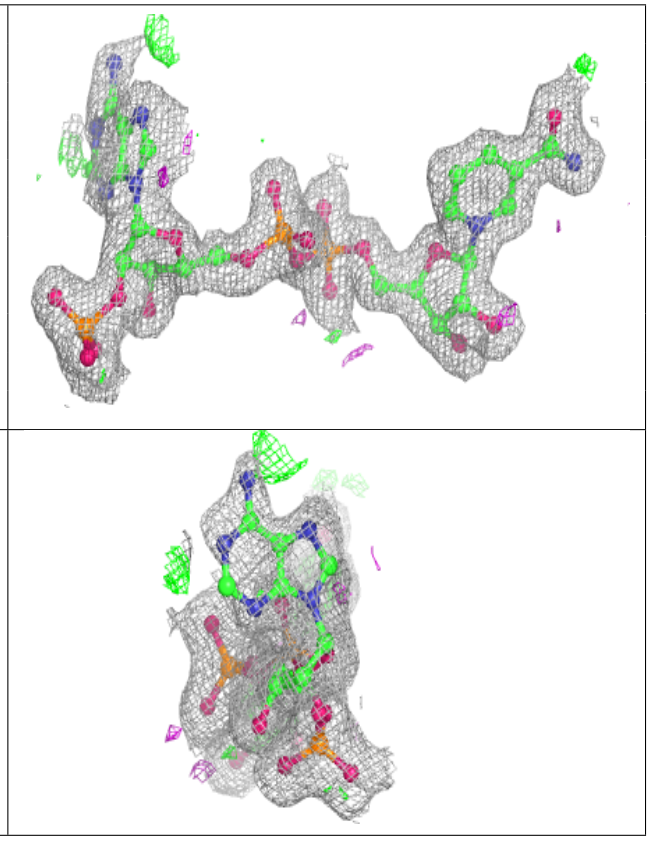
Electron density around D16 B 530:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



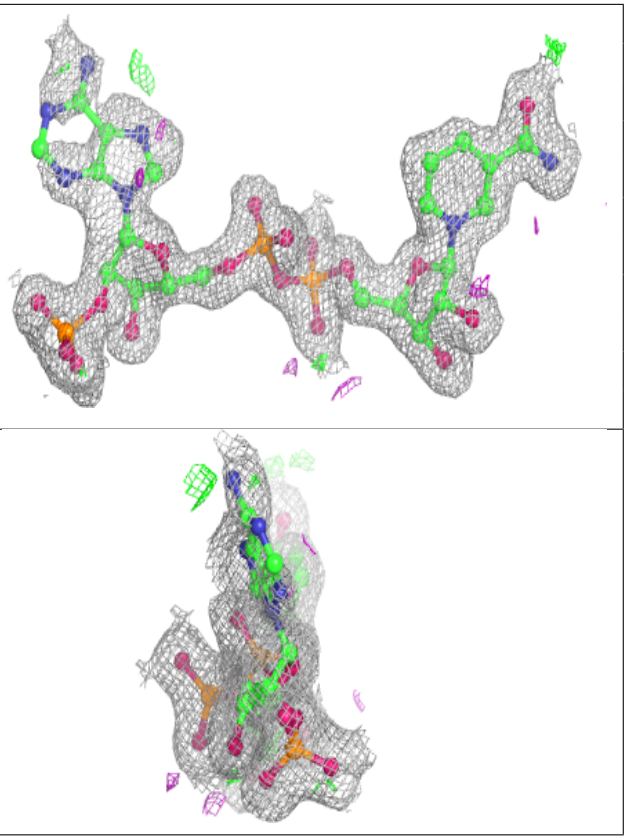
Electron density around NAP B 515 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



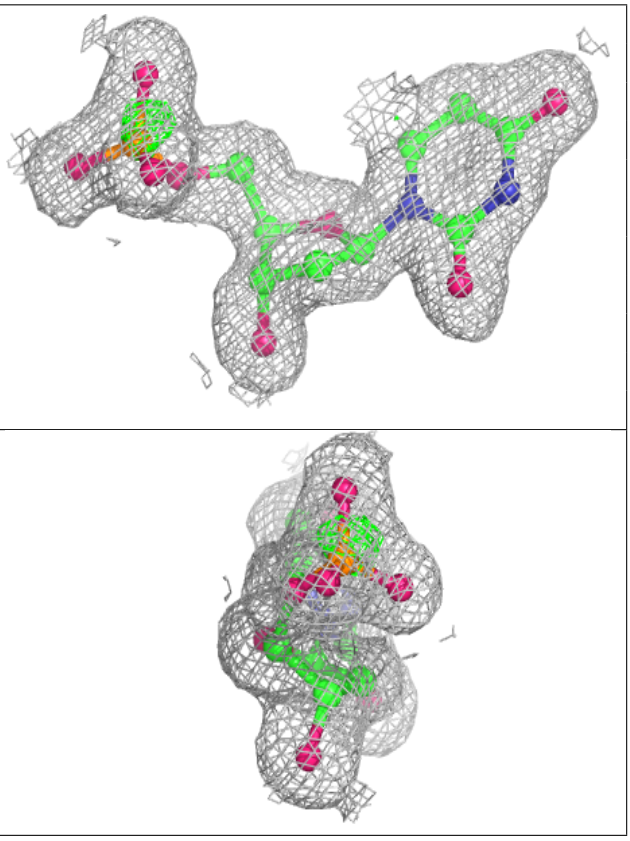
Electron density around NAP B 515 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UMP A 525:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UMP B 525:

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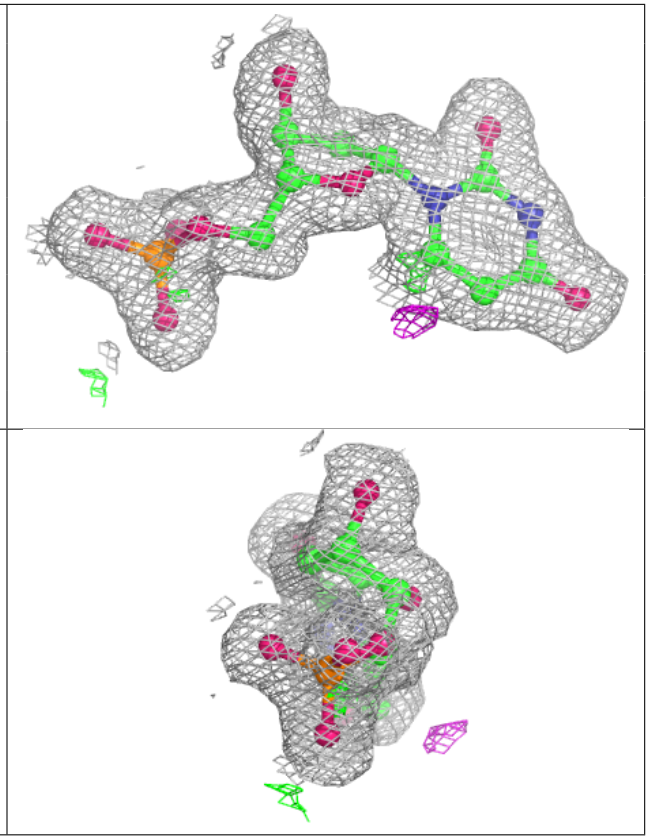
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.